

2,2,3,3,4,4,5,5,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid
15166-06-0 | DTXSID50562865

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.30 days

Global applicability domain: Outside

Local applicability domain index: 2.77e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

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Tetradeca-1,13-diene

Measured: 367

Predicted: 8.69

Image not found

Propylbenzene

Measured: 24.3

Predicted: 4.02

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1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17

Image not found

2-Methylheptane

Measured: 12.5

Predicted: 3.99

Image not found

2-Methylhexane

Measured: 12.5

Predicted: 5.54